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NEWS 25 MAR 11 ESBIOBASE reloaded and enhanced

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AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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STRUCTURE FILE UPDATES: 15 MAR 2009 HIGHEST RN 1121544-94-2
DICTIONARY FILE UPDATES: 15 MAR 2009 HIGHEST RN 1121544-94-2

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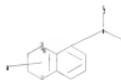
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chain nodes :

15 16 17 25 29 30

ring nodes :

1 2 3 4 5 6 7 8 9 10 18 19 20 21 22 23

chain bonds :

7-15 15-16 15-29 16-17 16-19 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 18-19 18-23 19-20 20-21
21-22 22-23

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 7-15 15-16 15-29 16-17 16-19 18-19 18-23 19-20
20-21 21-22 22-23 22-25

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 : 18 :

G1:C,N

G2:C,H

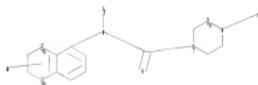
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15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:CLASS 29:CLASS 30:CLASS 31:Atom

L1 STRUCTURE UPLOADED

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chain nodes :

15 16 17 25 29 30

ring nodes :

1 2 3 4 5 6 7 8 9 10 18 19 20 21 22 23

chain bonds :

7-15 15-16 15-29 16-17 16-19 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 18-19 18-23 19-20 20-21
21-22 22-23

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 7-15 15-16 15-29 16-17 16-19 18-19 18-23 19-20
20-21 21-22 22-23 22-25

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 : 18 :

G1:C,N

G2:C,H

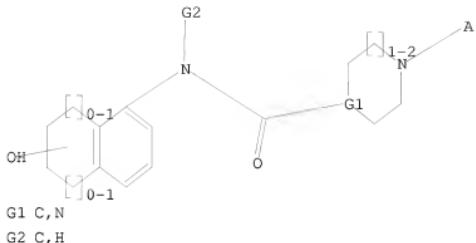
Match level :

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15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:CLASS 29:CLASS 30:CLASS 31:Atom

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s 11 full
FULL SEARCH INITIATED 18:59:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 127704 TO ITERATE
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100.0% PROCESSED	127704 ITERATIONS	17 ANSWERS
SEARCH TIME:	00.00.05	

L2 17 SEA SSS FUL L1

=> file caplus		SINCE FILE	TOTAL
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FILE COVERS 1907 - 16 Mar 2009 VOL 150 ISS 12
 FILE LAST UPDATED: 15 Mar 2009 (20090315/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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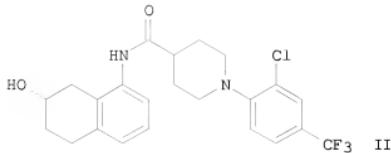
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2 full
L3 1 L2

=> d ibib abs hitstr tot

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:395272 CAPLUS
 DOCUMENT NUMBER: 142:447019
 TITLE: Preparation of tetrahydronaphthalene and urea derivatives as VR1 antagonists for the prophylaxis and treatment of diseases associated with VR1 activity, such as urological diseases, pain and inflammatory diseases
 INVENTOR(S): Bouchon, Axel; Diedrichs, Nicole; Hermann, Achim; Lustig, Clemens; Meier, Heinrich; Pernerstorfer, Josef; Reissmueller, Elke; De Vry, Jean; Mogi, Muneto; Urbahns, Klaus; Yura, Takeshi; Fujishima, Hiroshi; Tajimi, Masaomi; Yamamoto, Noriyuki; Yuasa, Hiroaki; Gupta, Jang; Tsukimi, Yasuhiro; Hayashi, Fumihiro
 PATENT ASSIGNEE(S): Bayer Healthcare Ag, Germany
 SOURCE: PCT Int. Appl., 76 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040119	A1	20050506	WO 2004-EP10606	20040922
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2540647	A1	20050506	CA 2004-2540647	20040922
EP 1670761	A1	20060621	EP 2004-765478	20040922
EP 1670761	B1	20090128		
R: DE, ES, FR, GB, IT				
JP 2007508255	T	20070405	JP 2006-530003	20040922
US 20070167458	A1	20070719	US 2006-574122	20061122
PRIORITY APPLN. INFO.:				
			EP 2003-22235	A 20031001
			EP 2003-25570	A 20031108
			WO 2004-EP10606	W 20040922
OTHER SOURCE(S): GI	CASREACT 142:447019; MARPAT 142:447019			



AB This invention relates to title compds. of formula A-NH-CO-E (I) [wherein A = 7-hydroxy-5,6,7,8-tetrahydronaphthalen-1-yl, 5,6-(un)substituted naphthalen-1-yl, indan-1-yl, etc.; E = (un)substituted piperidin-4-yl, piperazin-4-yl] and tautomeric or stereoisomers and salts thereof, which are useful as active ingredients of pharmaceutical prepsn. I have been synthesized as VR1 antagonists, and can be used for the prophylaxis and treatment of diseases associated with VR1 activity, in particular for the treatment of urol. disorders or diseases, pain and inflammatory disorders or diseases. Thus, acylation of ((7S)-7-Hydroxy-5,6,7,8-tetrahydronaphthalen-1-yl)amine with 1-(2-Chloro-4-trifluoromethylphenyl)piperidine-4-carboxylic acid gave II in 28% yield. The effects of the compds. were examined in the following several assays and pharmacol. tests: measurement of capsaicin-induced Ca²⁺ influx in a human VR1-transfected CHO cell line and in primary cultured rat dorsal root ganglia neurons, resp., measurement of capsaicin-induced bladder contraction, measurement of overactive bladder in anesthetized cystitis rats, measurement of acute pain, persistent pain, neuropathic pain, inflammatory pain and diabetic neuropathic pain (only the first assay had data). II showed an IC₅₀ ≤ 0.1 μM in the first assay. Specifically disclosed applications of I include the treatment of detrusor overactivity (overactive bladder), urinary incontinence, neurogenic detrusor overactivity (detrusor hyperflexia), idiopathic detrusor overactivity (detrusor instability), benign prostatic hyperplasia, and lower urinary tract symptoms; chronic pain, neuropathic pain, postoperative pain, rheumatoid arthritic pain, neuralgia, neuropathies, algesia, nerve injury, ischemia, neurodegeneration, stroke, and inflammatory disorders such as asthma and chronic obstructive pulmonary (or airways) disease (COPD).

IT
1044165-60-7 1044165-66-3 1044165-74-3
1044165-75-4 1044165-84-5 1044165-91-4
1044165-93-6 1044165-94-7 1044166-12-2
1044166-15-5 1044166-18-8 1044166-31-5
1044166-32-6 1044166-33-7 1044166-34-8
1044166-43-9 1044166-45-1

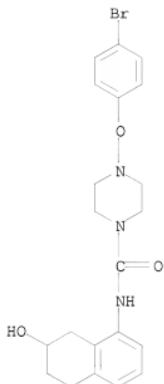
RL: PRPH (Prophetic)

(Preparation of tetrahydronaphthalene and urea derivatives as VR1 antagonists for the prophylaxis and treatment of diseases associated with VR1 activity, such as urological diseases, pain and inflammatory diseases)

RN 1044165-60-7 CAPLUS

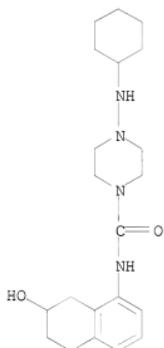
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RN 1044165-66-3 CAPLUS

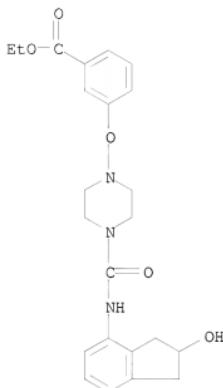
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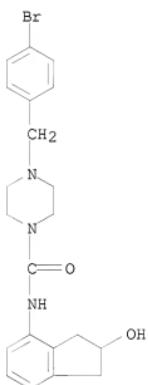
RN 1044165-74-3 CAPLUS

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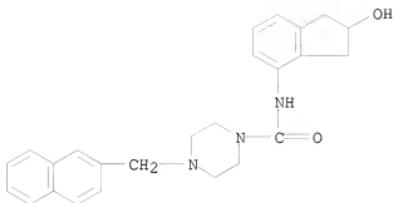


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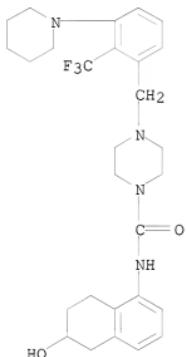


RN 1044165-84-5 CAPLUS
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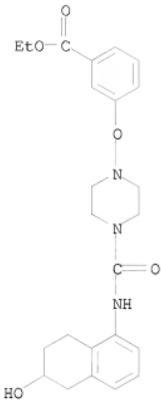
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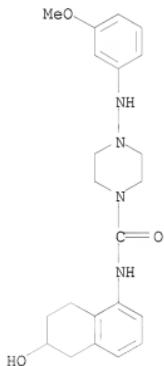
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CN INDEX NAME NOT YET ASSIGNED

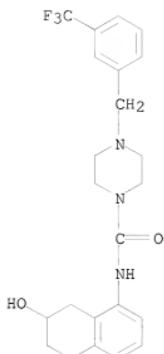


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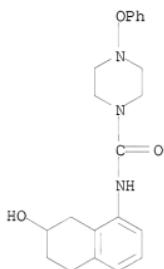


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10/513699

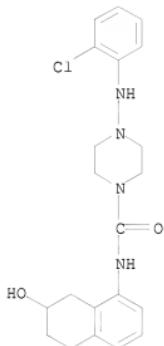


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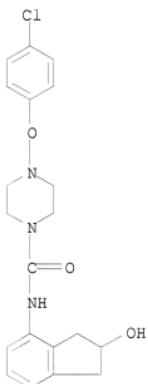


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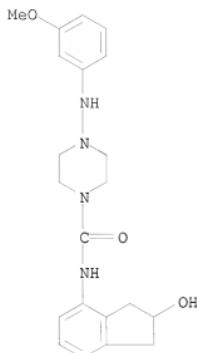


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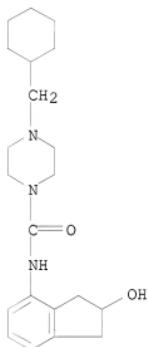


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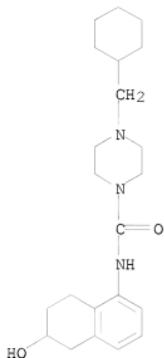
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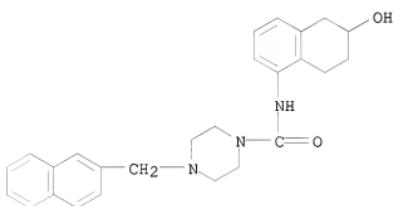
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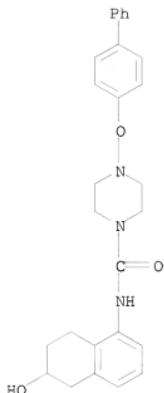
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RN 1044166-43-9 CAPLUS
CN 1-Piperazinecarboxamide, 4-(2-naphthalenylmethyl)-N-(5,6,7,8-tetrahydro-6-hydroxy-1-naphthalenyl)- (CA INDEX NAME)



RN 1044166-45-1 CAPLUS
CN 1-Piperazinecarboxamide, 4-((1,1'-biphenyl)-4-yloxy)-N-(5,6,7,8-tetrahydro-6-hydroxy-1-naphthalenyl)- (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1 STRUCTURE uploaded
L2 17 S L1 FULL

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L3 1 S L2 FULL

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